

PDE extension

Changes over Levon's extension

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New extension is compared to Levon's work ([2]), mostly chapter 4

Domains Geometry Definition

Originally

see [2] – 4.3.1.1 and 4.3.1.2

Saldamli defines domain shape by listing its boundaries. Individual boundaries (points in 1D, curves in 2D resp. surfaces in 3D) are describes by shape-functions. Shape-function maps intervals $([0,1]$ for curves, $[0,1] \times [0,1]$ for surfaces) onto the boundary.

Example half-circular domain according to [2]:

```
class Arc
  extends Boundary(ndims=2);
  parameter Point c = {0,0};
  parameter Real r = 1;
  parameter Real a_start = 0;
  parameter Real a_end = 2*Pi;
  redeclare function shape
    input Real tau;          //tau in [0,1]
    output Real coord[2];
  algorithm
    coord := c + r * { cos(a_start + (a_end - a_start) * tau),
                      sin(a_start + (a_end - a_start) * tau) };
  end shape;
end Arc;
```

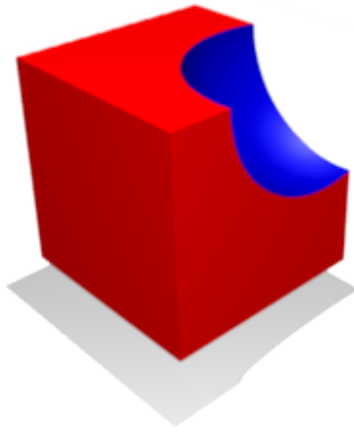


Figure 0.1: Boundary in 3D

```

class Line
  extends Boundary(ndims=2);
  parameter Point p1 = {0,0};
  parameter Point p2 = {1,0};
  redeclare function shape
    input Real h;          //h in [0,1]
    output Real coord[2];
  algorithm
    coord := p1 + (p2 - p1) * h;
  end shape;
end Line;

type Half-circularDomain
  extends Cartesian2D(boundary = {arc, line});
  parameter Arc arc (c = {0,0}, r = 2, a_start = Pi/2, a_end =
Pi*3/2);
  parameter Line line (p1 = {0,-2}, p2 = {0,2});
end Half-circularDomain;

```

Problem

This approach doesn't work well in 3D: if boundary is composed of several surfaces, parameters (arguments) of shape-function of these surfaces must be bounded not just in $[0, 1] \times [0, 1]$ interval but in some more complex set for each boundary surface so that they form a continuous boundary, e.g. see fig. 0.1. And there is no way to write this in Levon's extension.

Even if the syntax allowed this, it would be difficult for the user to compute these sets where parameters are bounded.

There is also no simple way to generate grid points during translation/solution.

Alternative approach

According to Peter's book [1] – 8.5.2, we define interior and boundaries of domain (these elements are called *regions* here) with one shape-function and for each region specify intervals for the shape-function arguments. This approach isn't more general (actually less), but is consistent in 1, 2 and 3D and (to me) is more natural. Inner points may be generated using this shape-function.

Modified Domain built-in type:

```
type Domain
  parameter Integer ndims;
  Real cartesian[ndims];
  Real coord[ndims] = cartesian;
  replaceable Region interior;
  replaceable function shape
    input Real u[ndims];
    output Real coord[ndims];
  end shape;
end Domain;
```

Region built-in type instead of Boundary:

```
type Region
  parameter Integer ndims;    //dim of space
  parameter Integer ndimr;    //dim of region
  parameter Real[ndims][2] interval;
  replaceable function shape;
    input Real u[ndims];
    output Real coord[ndims];
  end shape;
end Region;
```

```
type Region1D
  extends Region(ndimr = 1);
end Region1D;
```

Example circular domain:

```

class DomainHalf-circle
  extends Domain;
  parameter Real radius = 2;
  parameter Real[2] c = {0,0};
  function shapeFunc
    input Real r,v;
    output Real coord[2];
  algorithm
    coord := c + radius * r * { cos(Pi*(1/2 + v),
                                sin(Pi*(1/2 + v) )};

  end shapeFunc;
  Region2D interior(shape = shapeFunc, interval = {{0,1},{0,1}});
  Region1D arc(shape = shapeFunc, interval = {1,{0,1}});
  Region1D line(shape = shapeFunc, interval = {{-1,1},0});
end DomainHalf-circle;

```

Shape-function is not a pure function and thus it is not supported in current Modelica. To avoid this problem modified version was designed:

Modified version

Shape-function is replaced by equation and parameters of shape-function by new general coordinate system (that may not have a good physical meaning for some domains) here:

```

class DomainHalf-circle
  extends Domain;
  parameter Real radius = 2;
  parameter Real[2] c = {0,0};
  Real r, v;
  Region2D interior(v in {0,1}, r in {0,1});
  Region1D arc(v in {0,1}, r = 1);
  Region1D line(v = 0, r in {-1,1});
equation
  //coordinate transformation equation:
  coord = c + radius * r * { cos(Pi*(1/2 + v), sin(Pi*(1/2 + v) )};
end DomainHalf-circle;

```

One of these approaches should be chosen.

More complex geometries

More complex geometries may be defined using *Constructive Solid Geometry* – it is applying union, intersection and difference on previously defined shapes. The syntax is not designed already. It should be also possible to define domain in external file from some CAD app.

Differential operators

4.3.2

Partial derivatives

Originally

see 4.3.2.1

e.g. $\frac{\partial u}{\partial t}$.. `der(u)`, $\frac{\partial^2 u}{\partial x \partial y}$.. `der(u,x,y)`

Problem

There is no way to write mixed time and space derivative $\frac{\partial^2 u}{\partial x \partial t}$ in this notation.

This notation doesn't agree with mathematics, where we have different operators for ordinary ($\frac{du}{dx}$) and partial ($\frac{\partial u}{\partial x}$) derivatives.

`der(u)` for partial time derivative is confusing.

Alternative approach

$\frac{\partial u}{\partial t}$.. `pder(u,time)`

$\frac{\partial^2 u}{\partial x \partial y}$.. `pder(u,x,y)`

Now we can also write $\frac{\partial^2 u}{\partial x \partial t}$ as `pder(u,x,time)`

Normal derivative and normal vector

Originally

see 4.3.2.2

normal vector is implicit member of domain

Problem

Normal vector makes sense only in regions of dimension $n-1$ in n -dimensional domain (i.e. surface in 3D, curve in 2D and point in 1D). There is no normal vector in n dimensional region and infinitely many in less than $n-1$ dimensional regions.

Alternative approach

normal vector `n` is implicit member of all $n-1$ dimensional regions in n -dimensional domain. So we write

```
pder(u,omega.boundary.n) = 0 in omega.boundary;
```

A shorten notation is suggested in next section.

Using normal vector outside differential operators should be also possible e.g.:

```
field Real[3] flux;
```

```
flux*omega.boundary.n = 0 in omega.boundary;
```

Accessing coordinates and normal vector in `der()` operator

Originally

not discussed

Problem

Coordinates and normal vector are defined within the domain class, but they are used in equations that are written outside domains. Thus they should be accessed using `domainName. prefix` (e.g. `omega.x`), which is tedious.

In the example in 4.3.2.2 in [2] the normal vector `n` is reached outside the domain class without `domainName. prefix` even thou it is defined in the domain. It is not explained how this is enabled.

Solution

Fields are differentiated with respect to coordinates or normal vector only (or may be also some other vector for directional derivative??). Thus in place of second and following operands of `pder()` operator may be given only coordinates or normal vector. So variables in this positions may be treated specially and coordinates and normal vector of the domain of the field being differentiated may be accessed without the `domainName. prefix` here.

If coordinates or normal vector is used in different context (not in place of second and following operands of `pder()`), an alias for it may be defined in the model, e.g.

```
Real x = omega.x;
```

or (discussed later)

```
coordinate Real x = omega.x;
```

Perhaps usage of this shortened notation was intended even in the original extension but was not mentioned.

Start values of derivatives

Originally

not discussed

problem

Higher derivatives are allowed for fields thus we need to assign initial values to its derivatives sometimes.

solution

New attributes `startPrime` and `startSecond` (May be `startSecond` is not needed??) for field variables are introduced. Usage e.g.:

```
field Real u(start = 0, startPrime = field(sin(x*y) for (x,y) in omega);
```

Initial values for higher derivatives must be assigned in `initial equation` section.

Usage of `in` operator

PDEs

Originally

see 4.3.3

`in` operator is used for BCs to specify on which region they hold. It is not used for PDEs.

problem

PDEs hold on particular regions (usually `interior`) as well. Specification of region for BC but not for PDE is confusing. Besides that, the domain may be split into separate regions and different PDE may hold on each region.

solution

We suggest to use `in` operator also in PDEs to specify the region, as it is also in [1].

Accessing field values

Originally

see 4.2.4, in function-like style

problem

It is not consistent with current Modelica – to access values of regular variables in particular time in this function-like style is also not allowed.

If more than one coordinate system are defined in a domain (discussed later), it is not clear which coordinates are used in the function-like expression.

solution

Regions consisting of one point and the `in` operator will be used instead to represent the particular point. E.g.

```
model heatPID
  record Room extends DomainBlock3D;
    Region0D sensorPosition(shape = shapeFunc, range = {{1, 1}, {0.5, 0.5}, {0.5,
0.5}});
  end Room
  Room room(...)
  field Real T(domain = room);
  Real Ts;
  ...
equation
  Ts = T in room.sensorPosition;
  ...
end heatPID;
```

`in` operator will be probably used also to match regions from different domains and to write equations (boundary conditions) relating fields from different domains. The syntax is not developed yet.

Modifications presented below are not so important and are questionable.

Coordinates

Originally

see 4.3.1.1 and 4.3.1.3

There are two arrays for coordinates predefined in the built-in `Domain` type. `cartesian` for cartesian coordinates and `coord` for arbitrary coordinates specified by the user. No other coordinates may be defined except aliases to elements of these predefined arrays.

Problem

May be this is not flexible enough. User may need more different coordinate systems.

Solution

new modifier `coordinate` to define coordinates. Usage e.g.

```
"coordinate Real" coordName;
```

The array `coord` in the built-in `Domain` type may be left out then.

Field literal constructor

originally

see 4.2.2, e.g.:

```
u = field(2*a+b for (a,b) in omega)
```

where iterator variables `(a,b)` exist only in constructor expression and represent coordinates in `omega` (probably `coord`, but may be `cartesian`, it is not clear from the document.)

problem

It allows to define the field values in terms of only one coordinate system. There may be two (or more – if `coordinate` keyword admitted) coordinate systems defined and it may be useful to be able to define fields using any of them.

And the syntax suggested below is shorter and simpler anyway.

solution

modified syntax:

```
"field (" expr "in" dom ")"
```

or just shortcut

```
"{" expr "in" dom "}"
```

where `dom` is a domain and `expr` may depend on coordinates defined in this domain. E.g.


```
field Real f = field(2*omega.x+omega.y in omega.interior);
```

Further problems

How to write equations (mainly BC) connecting fields defined in different domains (some kind of distributed connectors)?

References

- [1] Peter Fritzson. *Principles of Object-Oriented Modeling and Simulation with Modelica 2.1*. Wiley-IEEE Press, 2004.
- [2] Levon Saldamli. *A High-Level Language for Modeling with Partial Differential Equations*. PhD thesis, Department of Computer and Information Science, Linköping University, 2006.